

Isoscaling, Symmetry Energy and Thermodynamic Models

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Abstract

The isoscaling parameter usually denoted by α depends upon both the symmetry energy coefficient and the isotopic contents of the dissociating systems. We compute α in theoretical models: first in a simple mean field model and then in thermodynamic models using both grand canonical and canonical ensembles. For finite systems the canonical ensemble is much more appropriate. The model values of α are compared with a much used standard formula. Next we turn to cases where in experiments, there are significant deviations from isoscaling. We show that in such cases, although the grand canonical model fails, the canonical model is capable of explaining the data.

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I. INTRODUCTION

For central collisions of Sn on Sn ($^{112}\text{Sn}+^{112}\text{Sn}$, $^{124}\text{Sn}+^{112}\text{Sn}$ and $^{124}\text{Sn}+^{124}\text{Sn}$) a well-known result is that the ratio of isotope yields from two different reactions, 1 and 2, $R_{21}(N, Z) = Y_2(N, Z)/Y_1(N, Z)$ exhibits an exponential relationship as a function of the isotope neutron number N and proton number Z [1, 2, 3]:

$$R_{21}(N, Z) = Y_2(N, Z)/Y_1(N, Z) = C \exp(\alpha N + \beta Z) \quad (1)$$

This is called isoscaling. Note that for Sn on Sn central collisions the fragmenting system is rather large. When the fragmenting system is significantly smaller, the above equation is only approximate [4]. We will confine ourselves to large systems till we come to sections VII and VIII.

Much effort has gone into trying to relate α to the symmetry energy term that occurs in liquid drop binding energy formula. In its simplest version the symmetry energy term is given by $C_s(N - Z)^2/A$. It is reasonable to guess that the ratio $R_{21}(N, Z)$ should predominantly depend on N_0, Z_0 or equivalently on Z_0, A_0 of the fragmenting systems and also on the value of C_s . An approximate functional relationship that can be deduced from models is: $\alpha \approx 4\frac{C_s}{T}((Z_0(1)/A_0(1))^2 - (Z_0(2)/A_0(2))^2)$ where $Z_0(1)/A_0(1)$ refers to the disassociating system in reaction 1, $Z_0(2)/A_0(2)$ refers to that in reaction 2 and T is the characteristic temperature in the two reactions. It is this approximate equality that we examine in this work, first in a mean-field model (section III) and then, in detail, in thermodynamic model using both canonical and grand canonical ensembles. In particular we point out a different functional relationship is more natural in certain physical situations. Next we turn to cases where isoscaling is only approximate and how such cases can be handled in the theoretical framework. Summary and conclusions are presented in section X.

II. RELATING ISOSCALING PARAMETER TO CHEMICAL POTENTIAL

Equation (1) can be easily understood using a grand canonical model for multifragmentation. This allows us to relate α to chemical potentials.

We assume that in a central collision, the two ions fuse, some pre-equilibrium emission occurs and the fused system, because of two-body collisions is heated up and begins to

expand. During the expansion composites are formed. As the expansion takes place interaction between composites rapidly fall off except for Coulomb interaction which can be taken care of in an approximate way using the Wigner-Seitz approximation [5]. In this expanded volume the break up of the dissociating system can be calculated using laws of equilibrium statistical mechanics. The calculation is particularly simple if a grand canonical ensemble is used.

More about the grand canonical approximation will follow later but at this stage let us quickly connect α to chemical potential encountered in the grand canonical ensemble. The cross-section of the produced composite is given by $\sigma(N, Z) = C \langle n_{N,Z} \rangle$ where C is a constant not provided by the model; $\langle n_{N,Z} \rangle$ is average multiplicity of the composite. For system 1 characterized by total charge $Z_0(1)$ and total mass $A_0(1)$ (total neutron number $N_0(1) = A_0(1) - Z_0(1)$) and neutron and proton chemical potentials $\mu_n(1)$ and $\mu_p(1)$ respectively this multiplicity is

$$\langle n_{N,Z}(1) \rangle = e^{\beta \mu_n(1)N + \beta \mu_p(1)Z} \omega_{N,Z} \quad (2)$$

where β is the inverse of temperature T and $\omega_{N,Z}$ is the one particle partition function of the composite N, Z .

If in the second reaction the total charge is $Z_0(2)$, the total mass is $A_0(2)$ but the conditions of the second reaction are similar to that of reaction 1 and we expect the same temperature, then

$$\frac{\sigma_2(N, Z)}{\sigma_1(N, Z)} \propto e^{\beta(\mu_n(2) - \mu_n(1))N + \beta(\mu_p(2) - \mu_p(1))Z} \quad (3)$$

as the $\omega(N, Z)$ in the numerator cancels the $\omega(N, Z)$ in the denominator. Let $\delta\mu_n \equiv \mu_n(2) - \mu_n(1)$ and $\delta\mu_p \equiv \mu_p(2) - \mu_p(1)$. A widely used relationship is

$$\delta\mu_n \approx 4c_s \left[\left(\frac{Z_0(1)}{A_0(1)} \right)^2 - \left(\frac{Z_0(2)}{A_0(2)} \right)^2 \right] \quad (4)$$

A corresponding relationship can be written down for $\delta\mu_p$. It suffices to study any one and traditionally one examines $\delta\mu_n$. In the following we will investigate $\delta\mu_n$ for various cases.

III. $\delta\mu_n$ IN A MEAN FIELD MODEL

The concept of chemical potential is useful not only in problems concerned with multifragmentation. We first investigate the chemical potential in mean field theory at finite

temperature. One might argue that this is a valid model at low temperatures $T \leq 3$ MeV. The caloric curve has been computed in this model [6, 7] and many interesting results were found.

For a nucleus with N neutrons and Z protons ($N + Z = A$) the symmetry energy contributes to the binding energy a term: $C_s \frac{(N-Z)^2}{(N+Z)}$. To binding energy per particle it gives $C_s \frac{(N-Z)^2}{A^2}$. The term C_s has its origin to both kinetic and potential energy per particle so we separate C_s into two parts: $C_s = C_s(k.e) + C_s(p.e)$.

We consider asymmetric nuclear matter where proton charges are switched off. We can calculate both $C_s(k.e)$ and $C_s(p.e)$ in the Hartree-Fock model interacting by Skyrme interaction. For an asymmetric nucleus ρ_n and ρ_p are different. We have

$$\begin{aligned}\rho &= \rho_n + \rho_p \\ \Delta &= \frac{\rho_n - \rho_p}{\rho_n + \rho_p} = \frac{(N - Z)}{N + Z} = 1 - \frac{2Z}{A} \\ \rho_n &= \frac{\rho}{2}(1 + \Delta) \\ \rho_p &= \frac{\rho}{2}(1 - \Delta)\end{aligned}$$

In the Hartree-Fock model at zero temperature, the kinetic energy per nucleon is given by

$$\begin{aligned}\frac{K.E.}{A} &= \frac{N}{A} \frac{3}{5} \frac{p_f^2(n)}{2m} + \frac{Z}{A} \frac{3}{5} \frac{p_f^2(p)}{2m} \\ &= \frac{\rho_n}{\rho} \frac{3h^2}{10m} \left(\frac{3\rho_n}{8\pi}\right)^{2/3} + \frac{\rho_p}{\rho} \frac{3h^2}{10m} \left(\frac{3\rho_p}{8\pi}\right)^{2/3}\end{aligned}\quad (5)$$

Expanding the above in powers of Δ upto Δ^2 we get

$$\frac{K.E.}{A} = \frac{3}{10m} h^2 \left(\frac{3\rho}{16\pi}\right)^{2/3} \left(1 + \frac{5}{9} \Delta^2\right) \quad (6)$$

This then identifies $C_s(k.e)$:

$$C_s(k.e) = \frac{h^2}{6m} \left(\frac{3\rho}{16\pi}\right)^{2/3} \quad (7)$$

Of course, in $\frac{K.E.}{A}$ terms of higher powers of Δ exist which will be small and are neglected.

For contribution $C_s(p.e)$ we start with the simplest potential energy density that will produce the correct saturation density, binding energy, compressibility and symmetry energy coefficient [8]:

$$V(\rho_n, \rho_p) = \frac{A_u}{\rho_0} \rho_n \rho_p + \frac{A_l}{2\rho_0} (\rho_n^2 + \rho_p^2) + \frac{B}{\sigma + 1} \frac{\rho^{\sigma+1}}{\rho_0^\sigma} \quad (8)$$

This will give for potential energy per particle:

$$\frac{P.E.}{A} = A_u \frac{\rho_n \rho_p}{\rho \rho_0} + \frac{A_l}{2\rho \rho_0} (\rho_n^2 + \rho_p^2) + \frac{B}{\sigma + 1} \left(\frac{\rho}{\rho_0}\right)^\sigma \quad (9)$$

Writing ρ_n, ρ_p in terms of ρ and Δ we get

$$\frac{P.E.}{A} = \frac{1}{4} \frac{\rho}{\rho_0} (A_u + A_l) + \frac{1}{4} \frac{\rho}{\rho_0} (A_l - A_u) \Delta^2 + \frac{B}{\sigma + 1} \left(\frac{\rho}{\rho_0}\right)^\sigma \quad (10)$$

We identify $C_s(p.e) = \frac{1}{4} \frac{\rho}{\rho_0} (A_l - A_u)$. With $A_u = -379.2 \text{ MeV}$, $A_l = -334.4 \text{ MeV}$, $B=303.9 \text{ MeV}$ and $\sigma=7/6$, one gets for symmetric nuclear matter saturation density $\rho_0 = 0.16 \text{ fm}^{-3}$, $B.E./A=16 \text{ MeV}$, compressibility=210 MeV and at $\rho/\rho_0=1$, $C_s(p.e)=11.2 \text{ MeV}$. Together with $C_s(k.e) \approx 12.3 \text{ MeV}$ C_s adds to the total value of 23.5 MeV.

The Hartree-Fock energy of an orbital is given by

$$\epsilon = p^2/2m + A_u(\rho_u/\rho_0) + A_l(\rho_l/\rho_0) + B(\rho/\rho_0)^\sigma \quad (11)$$

The value of μ_n is found by solving for a given ρ_n and $\beta = 1/T$

$$\rho_n = \frac{8\pi}{h^3} \int_0^\infty \frac{p^2 dp}{\exp[\beta(\epsilon_n - \mu_n)] + 1} \quad (12)$$

In the model pursued here, the potential part in ϵ is constant for given densities and is given by $K = \frac{\rho}{2\rho_0} (A_u + A_l) + \frac{\rho(A_l - A_u)}{2\rho_0} \Delta + B(\frac{\rho}{\rho_0})^\sigma = \frac{\rho}{2\rho_0} (A_u + A_l) + 2C_s(p.e)\Delta + B(\frac{\rho}{\rho_0})^\sigma$. For zero temperature, the chemical potential (at zero temperature $\mu = \epsilon_f$) is $\mu = \frac{p_f^2}{2m} + K$. We first consider zero temperature. This will be followed by the finite temperature case.

The change in neutron chemical potentials for two nuclei: one with $\Delta_2 = 1 - \frac{2Z_2}{A_2}$ and another with $\Delta_1 = 1 - \frac{2Z_1}{A_1}$ is

$$\delta\mu_n = \mu_n(2) - \mu_n(1) = \frac{p_f^2(n)}{2m}(2) - \frac{p_f^2(n)}{2m}(1) + 4C_s(p.e)\left(\frac{Z_1}{A_1} - \frac{Z_2}{A_2}\right) \quad (13)$$

The kinetic term is:

$$\frac{p_f^2(n)}{2m}(2) - \frac{p_f^2(n)}{2m}(1) = \frac{h^2}{2m} \left(\frac{3}{8\pi}\right)^{2/3} \left[\left(\frac{\rho}{2}\right)^{2/3} (1 + \Delta_2)^{2/3} - \left(\frac{\rho}{2}\right)^{2/3} (1 + \Delta_1)^{2/3}\right] \quad (14)$$

Expanding the above to the lowest order in Δ

$$\frac{p_f^2(n)}{2m}(2) - \frac{p_f^2(n)}{2m}(1) \approx \frac{h^2}{6m} \left(\frac{3\rho}{16\pi}\right)^{2/3} 4\left(\frac{Z_1}{A_1} - \frac{Z_2}{A_2}\right) \quad (15)$$

Together then we get

$$\delta\mu_n \approx 4.0 * C_s \left(\frac{Z_1}{A_1} - \frac{Z_2}{A_2}\right) \quad (16)$$

the approximate nature of the above equation arises because contributions from kinetic energy have been retained to lowest orders in Δ . Note the difference of the above equation from the generally used relation of eq.(4).

Consider now finite temperature mean field theory. The contribution to $\delta\mu_n$ from potential energy does not change. But the contribution to $\delta\mu_n$ from kinetic energy will change. An approximate answer, quite accurate upto 6 MeV temperature, is $[\frac{p_f^2(n)}{2m}(2) - \frac{p_f^2(n)}{2m}(1)](1 + \frac{\pi^2 T^2}{12e_0(1)e_0(2)})$ with $e_0(1) = \frac{p_f^2(n)}{2m}(1)$ and $e_0(2) = \frac{p_f^2(n)}{2m}(2)$. But it is easy to get an accurate answer for all temperatures numerically. Fig.1 shows that in this model eq.(16) works better than eq.(4).

One can do refinements to this model. For example as the temperature increases, the nucleus will expand [6, 7] which will cause some quantitative changes. But we will not pursue these finer details.

IV. $\delta\mu_n$ IN THERMODYNAMIC MULTIFRAGMENTATION MODELS: CANONICAL AND GRANDCANONICAL

We now go back to the multifragmentation model that we briefly alluded to in section II. Assume that the system with A_0 nucleons and Z_0 protons has temperature T , has expanded to a higher than normal volume and the partitioning into different composites can be calculated according to equilibrium statistical mechanics. In a canonical model, the partitioning is done such that all partitions have the correct A_0, Z_0 (equivalently N_0, Z_0). Details of the implementation of the canonical model can be found elsewhere [9]; here we give the essentials necessary to follow the present work.

The canonical partition function is given by

$$Q_{N_0, Z_0} = \sum \prod \frac{\omega_{I,J}^{n_{I,J}}}{n_{I,J}!} \quad (17)$$

Here the sum is over all possible channels of break-up (the number of such channels is enormous) which satisfy $N_0 = \sum I \times n_{I,J}$ and $Z_0 = \sum J \times n_{I,J}$; $\omega_{I,J}$ is the partition function of one composite with neutron number I and proton number J respectively and $n_{I,J}$ is the number of this composite in the given channel. The one-body partition function $\omega_{I,J}$ is a product of two parts: one arising from the translational motion of the composite and another

from the intrinsic partition function of the composite:

$$\omega_{I,J} = \frac{V_f}{h^3} (2\pi m T)^{3/2} A^{3/2} \times z_{I,J}(int) \quad (18)$$

Here $A = I + J$ is the mass number of the composite and V_f is the volume available for translational motion; V_f will be less than V , the volume to which the system has expanded at break up. We use $V_f = V - V_0$, where V_0 is the normal volume of nucleus with Z_0 protons and N_0 neutrons. In this calculation we have used a fairly typical value $V = 6V_0$.

The probability of a given channel $P(\vec{n}_{I,J}) \equiv P(n_{0,1}, n_{1,0}, n_{1,1}, \dots, n_{I,J}, \dots)$ is given by

$$P(\vec{n}_{I,J}) = \frac{1}{Q_{N_0, Z_0}} \prod \frac{\omega_{I,J}^{n_{I,J}}}{n_{I,J}!} \quad (19)$$

The average number of composites with I neutrons and J protons is seen easily from the above equation to be

$$\langle n_{I,J} \rangle = \omega_{I,J} \frac{Q_{N_0-I, Z_0-J}}{Q_{N_0, Z_0}} \quad (20)$$

The constraints $N_0 = \sum I \times n_{I,J}$ and $Z_0 = \sum J \times n_{I,J}$ can be used to obtain different looking but equivalent recursion relations for partition functions. For example

$$Q_{N_0, Z_0} = \frac{1}{N_0} \sum_{I,J} I \omega_{I,J} Q_{N_0-I, Z_0-J} \quad (21)$$

These recursion relations allow one to calculate Q_{N_0, Z_0}

We list now the properties of the composites used in this work. The proton and the neutron are fundamental building blocks thus $z_{1,0}(int) = z_{0,1}(int) = 2$ where 2 takes care of the spin degeneracy. For deuteron, triton, ^3He and ^4He we use $z_{I,J}(int) = (2s_{I,J} + 1) \exp(-\beta E_{I,J}(gr))$ where $\beta = 1/T$, $E_{I,J}(gr)$ is the ground state energy of the composite and $(2s_{I,J} + 1)$ is the experimental spin degeneracy of the ground state. Excited states for these very low mass nuclei are not included. For mass number $A = 5$ and greater we use the liquid-drop formula. For nuclei in isolation, this reads ($A = I + J$)

$$z_{I,J}(int) = \exp \frac{1}{T} [W_0 A - \sigma(T) A^{2/3} - \kappa \frac{J^2}{A^{1/3}} - C_s \frac{(I - J)^2}{A} + \frac{T^2 A}{\epsilon_0}] \quad (22)$$

The derivation of this equation is given in several places [5, 9] so we will not repeat the arguments here. The expression includes the volume energy, the temperature dependent surface energy, the Coulomb energy and the symmetry energy. The term $\frac{T^2 A}{\epsilon_0}$ represents contribution from excited states since the composites are at a non-zero temperature.

For most of the calculations here the dissociating system is $N_0 = 93, Z_0 = 75, A_0 = 168$ for reaction 1. For reaction 2, the dissociating system is $N_0 = 111, Z_0 = 75, A_0 = 186$. These will represent $^{112}\text{Sn}+^{112}\text{Sn}$ central collisions and $^{124}\text{Sn}+^{124}\text{Sn}$ central collisions after pre-equilibrium particles are emitted. These two systems have received much attention in the past. We also have to state which nuclei are included in computing Q_{N_0, Z_0} (eq.(17)). For I, J , (the neutron and the proton number) we include a ridge along the line of stability. The liquid-drop formula above also gives neutron and proton drip lines and the results shown here include all nuclei within the boundaries.

The long range Coulomb interaction between different composites can be included in an approximation called the Wigner-Seitz approximation. We incorporate this following the scheme set up in [5].

Computations of observables with the canonical model can be done without an explicit use of a chemical potential. We can, however, compute the chemical potential using the thermodynamic identity $\mu = (\partial F / \partial n)_{V, T}$ [10]. We know the values of $Q_{N_0, Z_0}, Q_{N_0-1, Z_0}$ and Q_{N_0, Z_0-1} . Since free energy F is just $-T \ln Q$ we compute μ_n from $-T(\ln Q_{N_0, Z_0} - \ln Q_{N_0-1, Z_0})$ and μ_p from $-T(\ln Q_{N_0, Z_0} - \ln Q_{N_0, Z_0-1})$.

We now briefly review the grand canonical model. For finite systems such as considered here it is inferior to the canonical model but is easier to implement. If the numbers of neutrons and protons in the dissociating system are N_0 and Z_0 respectively, the ensemble contains not only these but many others but the average value can be constrained to be N_0 and Z_0 . The chemical potentials μ_n and μ_p serve to fix the average numbers. If the neutron chemical potential is μ_n and the proton chemical potential is μ_p , then statistical equilibrium implies that the chemical potential of a composite with N neutrons and Z protons is $\mu_n N + \mu_p Z$. The following are the relevant equations for us. The average number of composites with N neutrons and Z is

$$\langle n_{N, Z} \rangle = e^{\beta \mu_n N + \beta \mu_p Z} \omega_{N, Z} \quad (23)$$

There are two equations which determine μ_n and μ_p .

$$N_0 = \sum N e^{\beta \mu_n N + \beta \mu_p Z} \omega_{N, Z} \quad (24)$$

$$Z_0 = \sum Z e^{\beta \mu_n N + \beta \mu_p Z} \omega_{N, Z} \quad (25)$$

The sum here is over all nuclei within drip lines whose (N, Z) do not exceed (N_0, Z_0) since there can not be a composite whose N, Z exceed those of the system from which it emerges.

We want to point out the following feature of the grand canonical model. In all $\omega_{N,Z}$'s in the sum in the above two equations, there is one common value for V_f (see eq.(18)). We really solve for N_0/V_f and Z_0/V_f . The values of μ_n or μ_p will not change if we, say, double N_0, Z_0 and V_f simultaneously provided the number of terms in the sum is unaltered. We then might as well say that when we are solving the grand canonical equation we are really solving for an infinite system (because we know that fluctuations will become unimportant) but this infinite system can break up into only certain kinds of species as are included in the above two equations. Which composites are included in the sum is an important physical ingredient in the model but intensive quantities like β, μ depend not on N_0, Z_0 but on N_0/V_f and Z_0/V_f . To apply the grand canonical model to finite systems after solving for μ 's we plug in the value of V_f that would be appropriate for the system N_0, Z_0 . If the system which we are investigating is small, experimental data may show substantial deviations from the grand canonical model as we will verify later.

For later application, we will also use a slightly different version of the above equations [11]. We label two other chemical potentials: μ (fixes baryon number) and ν (fixes total charge):

$$A_0 = \sum A e^{\beta\mu A + \beta\nu Z} \tilde{\omega}_{A,Z} \quad (26)$$

$$Z_0 = \sum Z e^{\beta\mu A + \beta\nu Z} \tilde{\omega}_{A,Z} \quad (27)$$

Here $\mu = \mu_n$, $\nu = \mu_p - \mu$ and $\tilde{\omega}_{A,Z} = \omega_{N,Z}$ with $A = N + Z$.

For $A_0 = 168, Z_0 = 75$ and $A_0 = 186, Z_0 = 75$ the μ_n 's of the grand canonical model are compared with those derived from the canonical model in Fig.2. The values are very close. We also compare the $\delta\mu_n$ in the two models.

V. COMPUTATION OF $\delta\mu_n$ AS $T \rightarrow 0$

The computation of μ whether in canonical or grand canonical requires solving complicated equations. However it may simplify as $T \rightarrow 0$ (see also [11]). We try this in the canonical model first.

As $T \rightarrow 0$ the translational degree of freedom can be considered frozen. Let A_0, Z_0 be stable against spontaneous dissociation (if A_0, Z_0 is one of the nuclei within neutron and proton drip lines then it can not spontaneously decay into a neutron(proton) plus a daughter; usually the only other channel one needs to check is an alpha plus daughter). As $T \rightarrow 0$, the system will drop to the ground state of A_0, Z_0 and we will have (eq.(17)) $Q_{N_0, Z_0} \rightarrow \omega_{N_0, Z_0}$ with ω_{N_0, Z_0} now given by $\exp(-\frac{1}{T}E_{gr}(N_0, Z_0))$. Consequently we get $\mu_n(N_0, Z_0) = E_{gr}(N_0, Z_0) - E_{gr}(N_0 - 1, Z_0)$. This result is of course physically meaningful: $-\mu_n$ is simply the separation energy required to free a neutron from bound nucleus N_0, Z_0 . Thus

$$\mu_n(N_0, Z_0) = -W_0 + term1 + term2 \quad (28)$$

$$term1 = \sigma[A_0^{2/3} - (A_0 - 1)^{2/3}] + \kappa Z_0^2[A_0^{-1/3} - (A_0 - 1)^{-1/3}] \quad (29)$$

$$term2 = C_s[\frac{(N_0 - Z_0)^2}{A_0} - \frac{(N_0 - 1 - Z_0)^2}{A_0 - 1}] \quad (30)$$

For us $term2$ is of greater significance. It can be rewritten as

$$\begin{aligned} term2 &= C_s(1 - \frac{4Z_0^2}{A_0(A_0 - 1)}) \\ &\approx C_s(1 - \frac{4Z_0^2}{A_0^2}) \end{aligned} \quad (31)$$

For $\delta\mu_n$ we need to take the difference between two chemical potentials. $Term1$ of eq.(28) contributes little in the difference and thus we end up with familiar eq.(4), i.e., $\delta\mu_n = 4 * [(\frac{Z_1}{A_1})^2 - (\frac{Z_2}{A_2})^2]$.

Eq.(16) can also be obtained but as an approximation to eq.(30). We can rewrite eq.(30) as

$$term2 = 2C_s - C_s \frac{1 + 4Z_0}{A_0} - C_s \frac{(N_0 - Z_0 - 1)^2}{A_0(A_0 - 1)} \quad (32)$$

For the examples we are using, $A_0 = 168(186)$ and $Z_0 = 75$, the third term in the right hand side of the above equation is much less important than the second term. If we neglect the third term and as before also $term1$ we end up with eq.(16), i.e., $\delta\mu_n = 4 * (Z_1/A_1 - Z_2/A_2)$.

Let us see if we can get a sensible answer in the grand canonical model. We will use the the alternative forms eqs (26) and (27): μ controls the baryon number and ν the total charge. So long as we maintain the general form of eqs.(26) and (27), that is, include in the sum all particle stable nuclei with $A \leq A_0, Z \leq Z_0$ the limits of μ and ν are very difficult to obtain even at the zero temperature limit. In particular we can not have mutiplicity 1 in the

ground state of the dissociating system A_0, Z_0 and zero occupation in all other composites in the sum in eqs. (26) and (27) (see, however, [11]). Exclusive occupation in the ground state of A_0, Z_0 can be achieved in the canonical model but not in the grand canonical ensemble as this violates a fluctuation equation. We will deal with that equation but let us look at this first in a more pedestrian fashion. At zero temperature the translational degree can be considered frozen. From eqs. (26) and (27), to get multiplicity 1 we need $(\mu A_0 + \nu Z_0 - E_{gr}(A_0, Z_0)) \rightarrow 0$ as $\beta \rightarrow \infty$. This alone is not enough to determine μ or ν but we also require $\mu A_0 + \nu Z - E_{gr}(A_0, Z)$ to maximise at $Z = Z_0$ so that at other values of Z the difference is negative and occupation in Z 's other than Z_0 will go to 0 as $\beta \rightarrow \infty$. The maximisation condition gives [11]

$$\nu = -4C_s \frac{A_0 - 2Z_0}{A_0} + \kappa \frac{2Z_0}{A_0^{1/3}} \quad (33)$$

Having determined ν , the value of μ can be found from $\mu A_0 + \nu Z_0 - E_{gr}(A_0, Z_0) = 0$. This procedure ensures that $\mu A_0 + \nu Z - E_{gr}(A_0, Z)$ is negative for $Z < Z_0$ and hence as $\beta \rightarrow \infty$ the occupation in composites labelled by A_0, Z with $Z < Z_0$ will go to zero. But this does not guarantee that $\mu A + \nu Z - E_{gr}(A, Z)$ will be less than zero for all A 's less than A_0 with Z 's less than Z_0 that are in the sum of eqs. (26) and (27). In fact they are not all negative and whenever they are positive, multiplicities for those (A, Z) 's blow up. Another way of understanding this is to realise that for sole occupation in (A_0, Z_0) there are three conditions to be met: $\mu A + \nu Z - E_{gr}(A, Z)$ must (1) go to 0 at A_0, Z_0 , (2) must maximise as a function of Z at A_0, Z_0 and (3) must maximise as a function of A at A_0, Z_0 . With only two parameters μ and ν this can not be achieved.

We can also deduce the impossibility of exclusive occupation in the ground state of A_0, Z_0 from very general arguments about fluctuations. It is easy to prove this when there is only one kind of particle (eqs.(19) to (21) in [9]). With 2 kinds of particles, neutrons and protons and hence 2 chemical potentials μ and ν the notation gets complicated. Quite generally, the equation for the grand canonical partition function, when there are many species i which are non-interacting, is given by

$$Z_{gr.can} = \prod_i \left(\sum_{n_i=0}^{\infty} (e^{\beta \mu_i})^{n_i} z_{n_i}(i) \right) \quad (34)$$

In our case i stands for both a and z , the composite mass and charge; $z_{n_i}(i)$ is the canonical partition function of n_i particles of type i ; n_i goes from 0 to ∞ as we are constructing a

grand partition function. We have $\mu_i = \mu a + \nu z$. We need not specify the functional form of $z_{n_i}(i)$.

Eq.(34) can be rewritten as

$$Z_{gr.can} = \sum_{m=0}^{\infty} e^{\beta\mu m} \tilde{z}_m \quad (35)$$

where we have absorbed the factors $e^{\beta\nu z}$ in \tilde{z}_m which is quite complicated but it only contains partition functions with total particle number m . We clearly have (fluctuation equation):

$$\langle m^2 \rangle - \langle m \rangle^2 = \frac{1}{\beta^2} \frac{\partial^2}{\partial^2 \mu} \ln Z_{gr}. \quad (36)$$

In our case $\ln Z_{gr}$ is particularly simple:

$$\ln Z_{gr} = \sum e^{\beta\mu A + \beta\nu Z} \tilde{\omega}_{A,Z} \quad (37)$$

and

$$\frac{1}{\beta^2} \frac{\partial^2}{\partial^2 \mu} \ln Z_{gr} = \sum_{A=1, A_0} A^2 \langle n_A \rangle \quad (38)$$

If $\langle n_A \rangle = 1$ for $A = A_0$ and 0 for all others then $\langle m^2 \rangle - \langle m \rangle^2 = A_0^2$ but this contradicts the assumption that the only occupation is for $m = A_0$ in which case the fluctuations would have been 0.

In spite of this conceptual difficulty, the expression for μ_n derived from the grand canonical ensemble in [11] and that derived here from canonical ensemble are not that different. In particular $\delta\mu_n$ will be practically the same. For completeness we write the two, one after the other. That in [11] is

$$\mu_n = -W_0 + \frac{\sigma}{A_0^{1/3}} - \kappa \frac{Z_0^2}{A_0^{4/3}} + C_s [1 - (\frac{2Z_0}{A_0})^2] \quad (39)$$

whereas we get

$$\mu_n = -W_0 + \sigma [A_0^{2/3} - (A_0 - 1)^{2/3}] + \kappa Z_0^2 [A_0^{-1/3} - (A_0 - 1)^{-1/3}] + C_s [1 - (\frac{2Z_0}{A_0})^2] \quad (40)$$

VI. $\delta\mu_n$ IN MORE GENERAL CASE

The contribution of the symmetry energy to $\delta\mu_n$ in the more general case will be function of temperature and not a constant as implied in eq.(4). This can most readily be seen by

analytically deriving $\delta\mu_n$ at high temperature. Let us derive this in the canonical ensemble first. At very high temperature we will get only neutrons and protons and so eq.(17) becomes particularly simple:

$$Q_{N_0, Z_0} \rightarrow \frac{\omega_{1,0}^{N_0} \omega_{0,1}^{Z_0}}{N_0! Z_0!} \quad (41)$$

The formula $\mu_n = -T[\ln Q_{N_0, Z_0} - \ln Q_{N_0-1, Z_0}]$ leads to $\mu_n(N_0, Z_0) = -T \ln \frac{\omega_{1,0}}{N_0}$ and hence $\delta\mu_n = T \ln(N_2/N_1)$ and thus not a function of the symmetry energy at all. It is easy to verify that in this high temperature limit the grand canonical ensemble gives identical answers. From $T = 0$ towards a large value of T this must happen gradually and so $\delta\mu_n$ must be an evolving function of T .

We are unable to derive a simple formula for $\delta\mu_n$ for a general T . The reasons for this failure are obvious enough. Eqs.(24) and (25) are highly non-linear and thus the grand canonical ensemble provides no simple leads. The relevant equations for the canonical model are easy to compute on a computer but otherwise are quite non-transparent. In Fig.3 we show as a function of temperature (relates to beam energy of collision) numerical results for $\delta\mu_n$ for the two systems studied here. Two results are shown; one with $C_s = 23.5$ MeV and another with $C_s = 15$ MeV. Extracting the value of C_s from $\delta\mu_n$ using eq.(4) is difficult because of temperature and hence beam energy dependence. Notice that at high temperature, the curves obtained with different values of C_s approach one another. They will converge to one line which will rise linearly with T .

A very interesting aspect of the experimental data is the behavior of $\delta\mu_n$ when Z_2/A_2 varies for fixed Z_1/A_1 or vice versa. In the thermodynamic model this depends on the beam energy. There is no such dependence in eq.(4). The simple prediction of eq.(4) is compared with thermodynamic model predictions in Fig.4. In the model, for fixed Z_1/A_1 , $\delta\mu_n$ is still approximately linear with $(Z_2/A_2)^2$ although deviation can be seen by eye-estimation. It is also noticed that use of eq.(4) to estimate C_s from $\delta\mu_n$ will underestimate the value of C_s at low temperature (4 or 5 MeV) but will overestimate the value at high temperature, for example, at 7 MeV.

Experiments directly measure $\alpha = \beta\mu_n$ rather than μ_n and we plot α from the thermodynamic model as a function of temperature in Fig.5. We also obtain α from eq.(4) and compare. Eq.(4) gives a $1/T$ dependence but the fall with T is much slower in the thermodynamic model at higher temperature. In the thermodynamic model α would reach

asymptotically a constant value $\ln \frac{N_2}{N_1}$. This difference in behavior between the two predictions can be ascertained in experiments.

There has been much activity in recent times relating α to C_s [12, 13, 14]. An approximate derivation of eq.(4) from the expanding excited source (EES) model can be found in [3]. Attempts to obtain this from antisymmetrised molecular dynamics can be found in [15]. Temperature dependence of symmetry energy was discussed by Li and Chen [16].

VII. DEVIATION FROM ISOSCALING: EXPLANATION FROM CANONICAL MODEL

We now discuss isoscaling and possible deviations from it. It will become clear in this and the following section that, from the point of view of theory, isoscaling can work very well when N/N_0 and Z/Z_0 are small (≤ 0.35). Many experimental data fall in this range [1, 2, 3] and isoscaling is one robust feature to emerge in recent experimental intermediate energy heavy ion collisions. If we now extend these observations to larger composites deviations are to be expected. Will the grand canonical and canonical results for R_{21} always agree? The answer is no; it depends upon the size of the dissociating system (N_0, Z_0), more precisely, upon the fractions N/N_0 and Z/Z_0 . The grand canonical model always predicts isoscaling. In this model

$$\begin{aligned} R_{21} &= C \frac{\langle n_{N,Z}(2) \rangle}{\langle n_{N,Z}(1) \rangle} \\ &= C \exp(\alpha N + \beta Z) \end{aligned} \quad (42)$$

where we have used eq.(2) and the advantage that with similar beam conditions the factors $\omega_{N,Z}$ in the denominator and the numerator cancel each other out. Therefore, in the grand canonical approximation, the slopes of $\ln R_{21}$ as a function of N for fixed Z (a) will never deviate from a straight line and (b) for different fixed Z 's the slopes will not change. In many experiments where the sizes of the composites [4] encompass from small to large this is not true. In Fig.6 we compare some experimental data with a grand canonical calculation. Experimental details can be found in [4, 17, 18]. In the experiment, reaction 1 is ^{58}Ni on ^9Be and reaction 2 is ^{64}Ni on ^9Be . For the grand canonical calculation, for reaction 1 the dissociating system is taken to be $^{58}\text{Ni} + ^9\text{Be}$ ($N_0 = 35, Z_0 = 32$) and for reaction 2 the dissociating system is taken to be $^{64}\text{Ni} + ^9\text{Be}$ ($N_0 = 41, Z_0 = 32$). All composites between

drip lines are included as detailed in section IV with the highest values of N, Z terminating at N_0, Z_0 . The limitations of the grand canonical model are very obvious in the figure. The slopes of $\ln R_{21}$ differ from straight lines for large Z and as well the same slope for all Z does not fit. In these calculations the same temperature was assumed for all composites. The actual situation may be more complicated requiring a different temperature for higher composites. However the deviation from linearity will require even further complications if one insists on using the grand canonical model to fit the data. From the point of view of theory, however, for the emitting systems in these cases, the use of the grand canonical approximation for the emissions of heavier composites is not valid.

The canonical model does not impose these restrictions. Now (see eq.(20))

$$R_{21} = C \frac{Q_{N_0-N, Z_0-Z}(2)}{Q_{N_0, Z_0}(2)} / \frac{Q_{N_0-N, Z_0-Z}(1)}{Q_{N_0, Z_0}(1)} \quad (43)$$

This formula is not transparent at all but produces deviations from isoscaling for small systems.

Let us show the results of the canonical model calculation for the same case as above: Ni on Be. The parameters for the calculations are the same as used for the grand canonical model: the same temperature, the same freeze-out volume and the same composites included in building the respective partition functions. But the canonical calculations (Fig.7) are significantly different from the grand canonical results (Fig.6) and much closer to experimental data.

VIII. FURTHER OBSERVATIONS ABOUT DIFFERENCES BETWEEN THE CANONICAL AND GRAND CANONICAL RESULTS

Instead dealing directly with $R_{21} \propto \frac{\langle n_{N,Z}(2) \rangle}{\langle n_{N,Z}(1) \rangle}$ let us investigate a simpler task: that of relating $\langle n_{N,Z} \rangle$ in canonical with that in grand canonical. The formula for $\langle n_{N,Z} \rangle$, eq.(20), respects constancy of total neutron and proton numbers in the partition function and in this regard is superior to eq.(23). If N/N_0 or/and Z/Z_0 are not small (for some cases in Figs.6 and 7 they are ≥ 0.5), eq.(20) can give quite different results from those given by eq.(23). This is so even when the chemical potentials given by the two models are very close. If the chemical potentials in the two ensembles are nearly the same (as found in all our examples

so far) that merely guarantees that

$$\begin{aligned}\frac{Q_{N_0-1,Z_0}}{Q_{N_0,Z_0}} &\approx e^{\beta\mu_n} \\ \frac{Q_{N_0,Z_0-1}}{Q_{N_0,Z_0}} &\approx e^{\beta\mu_p}\end{aligned}\tag{44}$$

Here the left hand side is given by the canonical model (and leads to the definition of fugacity and chemical potential in the canonical model) and the right hand side is computed from the grand canonical model (eqs.(24) and (25)). However, for $\langle n_{N,Z} \rangle$ to be nearly the same in the two ensembles we require

$$\frac{Q_{N_0-N,Z_0-Z}}{Q_{N_0,Z_0}} \approx e^{\beta\mu_n N + \beta\mu_p Z}\tag{45}$$

We show below how the left hand side of the above equation can lead to the right hand side when N/N_0 and Z/Z_0 are small but are expected to deviate when they are not small. To proceed let us call $\frac{Q_{A-1,B}}{Q_{A,B}}$ =neutron fugacity of the system A, B and $\frac{Q_{A,B-1}}{Q_{A,B}}$ =proton fugacity of the system A, B . Rewrite the left hand side of eq.(45) as

$$\frac{Q_{N_0-N,Z_0-Z}}{Q_{N_0,Z_0}} = \frac{Q_{N_0-N,Z_0-Z}}{Q_{N_0,Z_0-Z}} \times \frac{Q_{N_0,Z_0-Z}}{Q_{N_0,Z_0}}\tag{46}$$

The first term on the right hand side can be rewritten as a product of N terms involving neutron fugacities and the second term as a product of Z terms involving proton fugacities.

$$\frac{Q_{N_0-N,Z_0-Z}}{Q_{N_0,Z_0-Z}} = \frac{Q_{N_0-N,Z_0-Z}}{Q_{N_0-N+1,Z_0-Z}} \frac{Q_{N_0-N+1,Z_0-Z}}{Q_{N_0-N+2,Z_0-Z}} \dots \frac{Q_{N_0-1,Z_0-Z}}{Q_{N_0,Z_0-Z}}\tag{47}$$

The first term in the right hand side of the above equation is the neutron fugacity of the system $N_0 - N + 1, Z_0 - Z$, the second term is the neutron fugacity of the system $N_0 - N + 2, Z_0 - Z$ and so on; finally ending with neutron fugacity of the system $N_0, Z_0 - Z$. If N is negligibly small compared to N_0 and also Z is negligibly small compared to Z_0 then each of these terms can be approximated by neutron fugacity of the system N_0, Z_0 (for $N \approx 20$ and $Z \approx 20$ in Fig.7, this leads to gross errors) leading to $(\frac{Q_{N_0-1,Z_0}}{Q_{N_0,Z_0}})^N$. Equating $\frac{Q_{N_0-1,Z_0}}{Q_{N_0,Z_0}}$ to $e^{\beta\mu_n}$ we get the factor $e^{\beta\mu_n N}$ of eq. (45). (Even this can introduce significant error for $N \approx 20$.) It is clear also how $e^{\beta\mu_p Z}$ can arise by resolving $\frac{Q_{N_0,Z_0-Z}}{Q_{N_0,Z_0}}$ into Z proton fugacities.

The connection between the two sides in eq. (45) can also be established using a saddle-point approximation [19] but we will not pursue this any further.

It then follows that although at low N, Z canonical and grand canonical calculations can agree they will diverge when N, Z grow. This is highlighted in Fig.8.

IX. DISCUSSION ABOUT SECONDARY DECAYS

Before comparing with data (as is done in Fig.7) one needs to investigate the effects of sequential decay on calculated R_{21} . The multiplicities $\langle n_{I,J} \rangle$ refer to populations of nuclei at finite temperatures. Nuclei at finite temperatures can decay by particle emissions and values of $\langle n_{I,J} \rangle$ will change. However, because one is comparing ratios, the effect on R_{21} may be less drastic. We have included the contributions from excited states through a factor $T^2 A / \epsilon_0$ in eq.(22). This overestimates contributions to the partition function from excited states and a cut-off will be necessary [20]. This requires detailed work which we have not carried out. In investigating isoscaling using antisymmetrised molecular dynamics, Ono et al. [21] find that the effect of secondary decay is to decrease α to $\alpha/2$. This means the experimental value of $\log R_{21}$ should be compared to $\log \sqrt{n(2)/n(1)}$ rather than to $\log[n(2)/n(1)]$. We have applied this “empirical” correction to the Ni on Be case in Fig.9. We now use temperature $T=5$ MeV. This leads to a steeper rise (compared to the $T=8$ MeV). But after the correction the rise decreases to a value more compatible with experiments. It now corresponds roughly to “uncorrected” $T=8$ MeV calculation.

X. SUMMARY

This work has addressed two issues. How well does eq.(4), a much used formula, fit results from calculations obtained from well-known models of nuclear dissociation? We find the fit approximately correct though not exact (the mean field model gives a different formula but the mean field model is not a model for multifragmentation). A more important question is: how do we handle cases when deviations from isoscaling are significant. Preliminary results reported here are very encouraging. Statistical multifragmentation can explain the results but one must give up using the grand canonical ensemble and instead use models that strictly conserve neutron and proton numbers.

XI. ACKNOWLEDGEMENT

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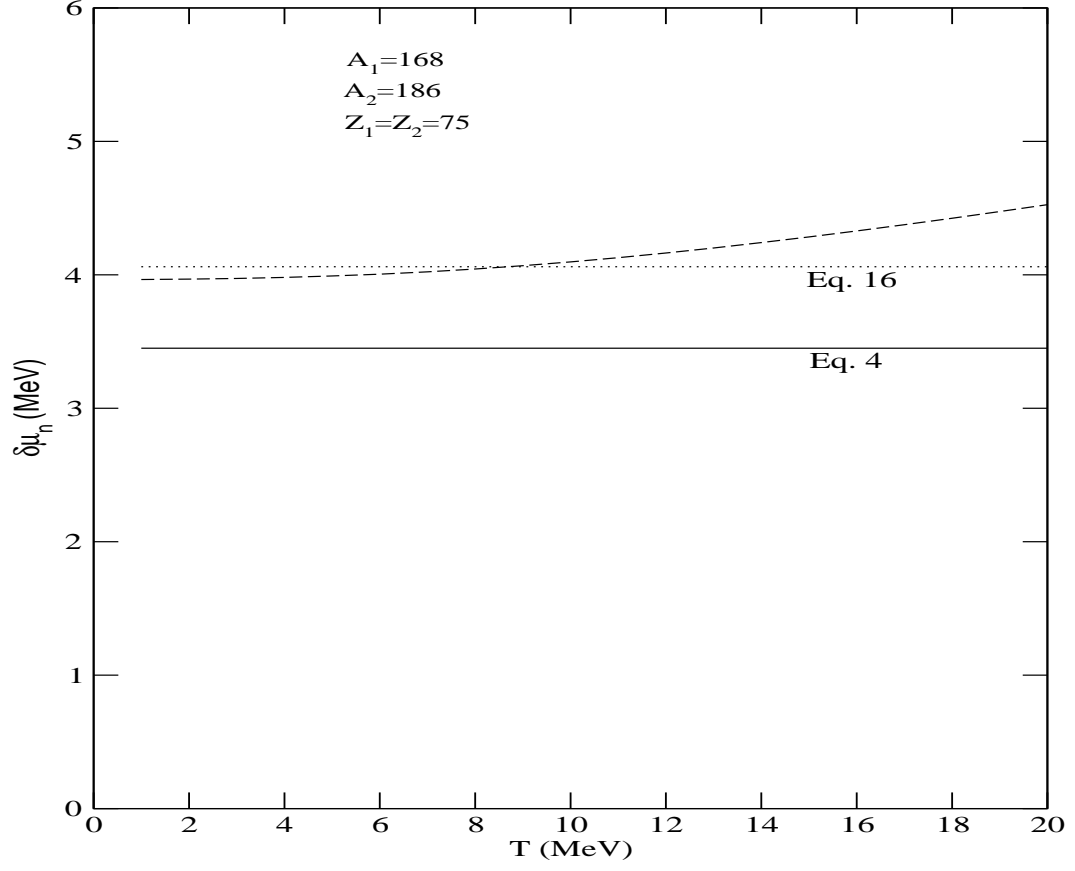


FIG. 1: Mean-field model calculation (dashed curve) for $\delta\mu_n$ compared with simple versions (eq.(16) and eq.(4)).

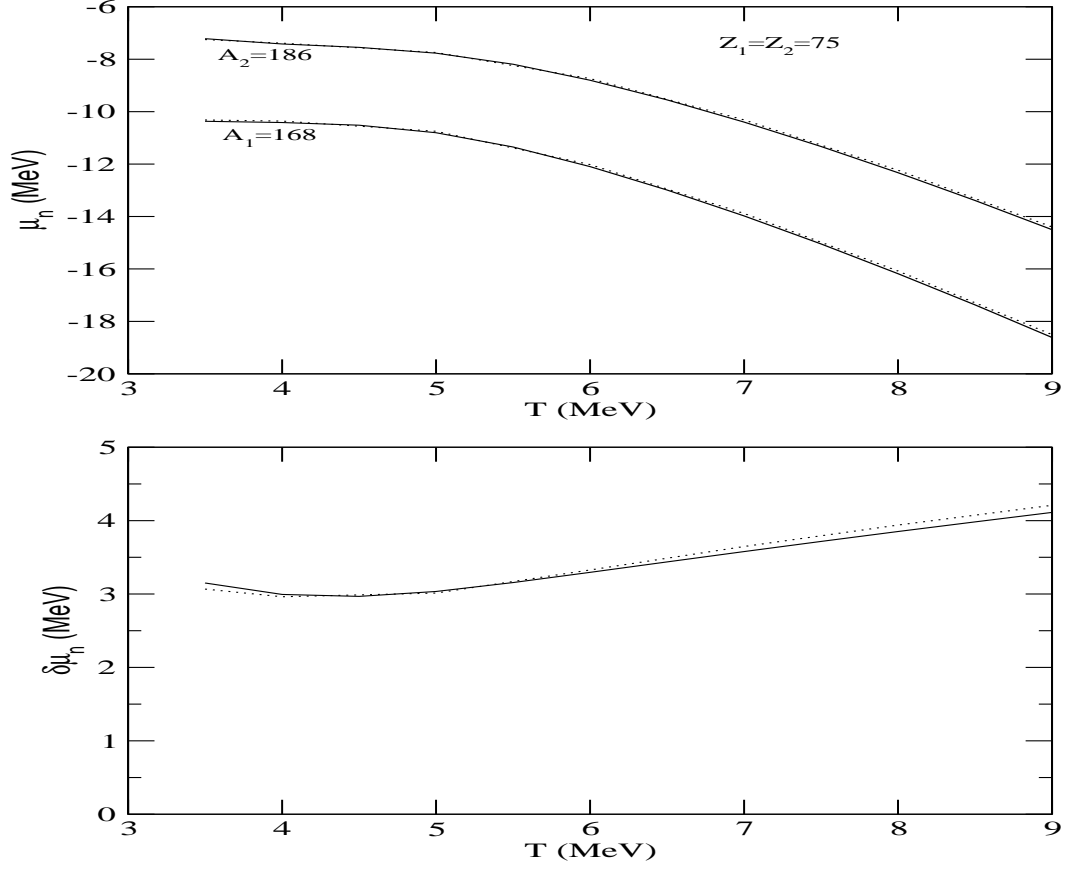


FIG. 2: Chemical potentials μ_n (top panel) for systems $Z_1 = 75, A_1 = 168$ and $Z_2 = 75, A_2 = 186$. Canonical model (dashed curve) and grand canonical model (solid line) results are quite close. The bottom panel shows results for $\delta\mu_n$ in a much more enlarged scale.

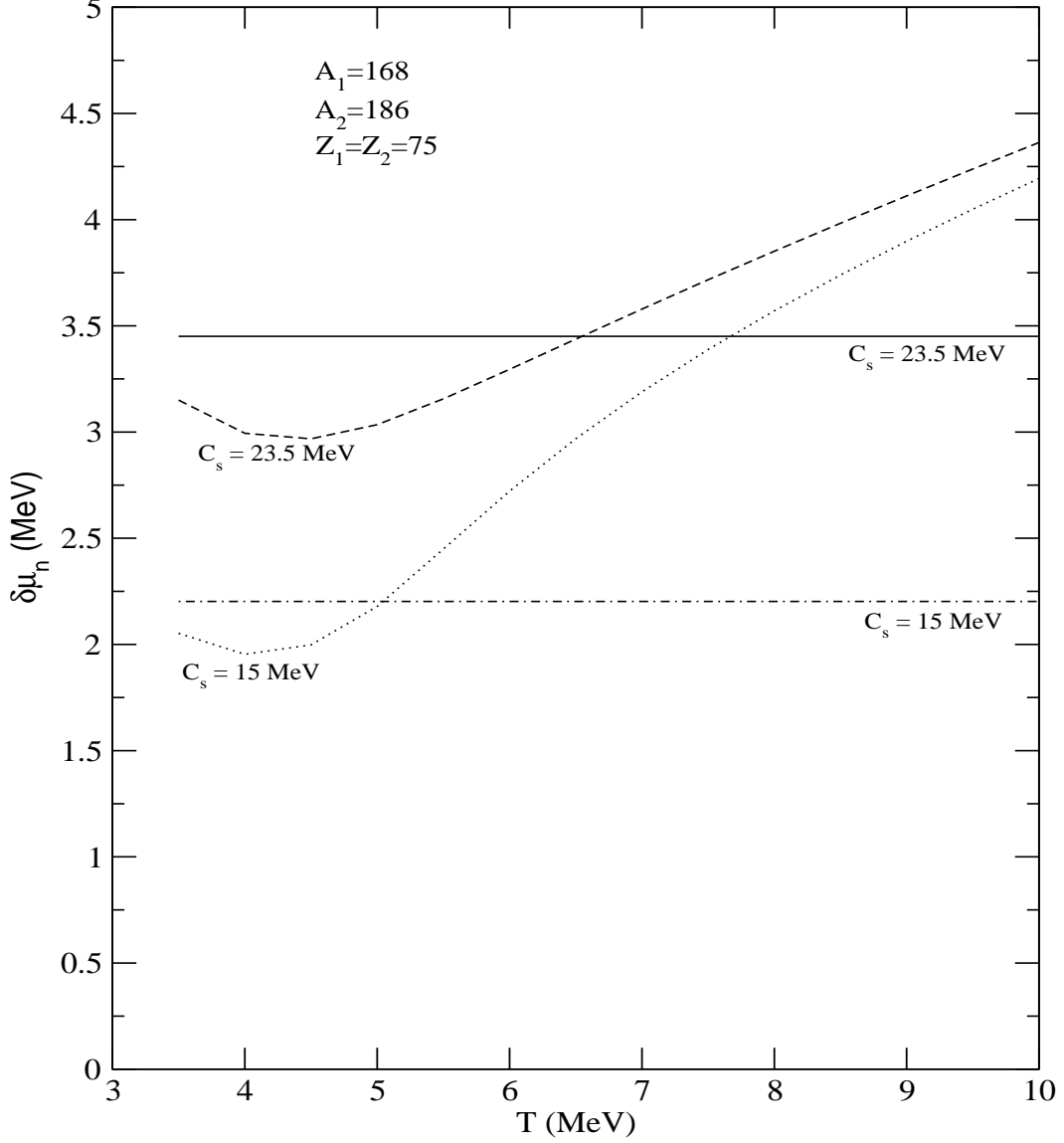


FIG. 3: The difference $\delta\mu_n$ calculated from theory compared with the simple prediction of eq.(4). Since canonical and grand canonical results for $\delta\mu_n$ are so close we just display the canonical model results. Two values of the symmetry energy coefficients were used. Notice that thermodynamic model predictions for $\delta\mu_n$ depend on the temperature unlike the simple model prediction (eq.(4)). In particular, irrespective of C_s , the theoretical value of $\delta\mu_n$ will approach the value $T \ln N_2/N_1$.

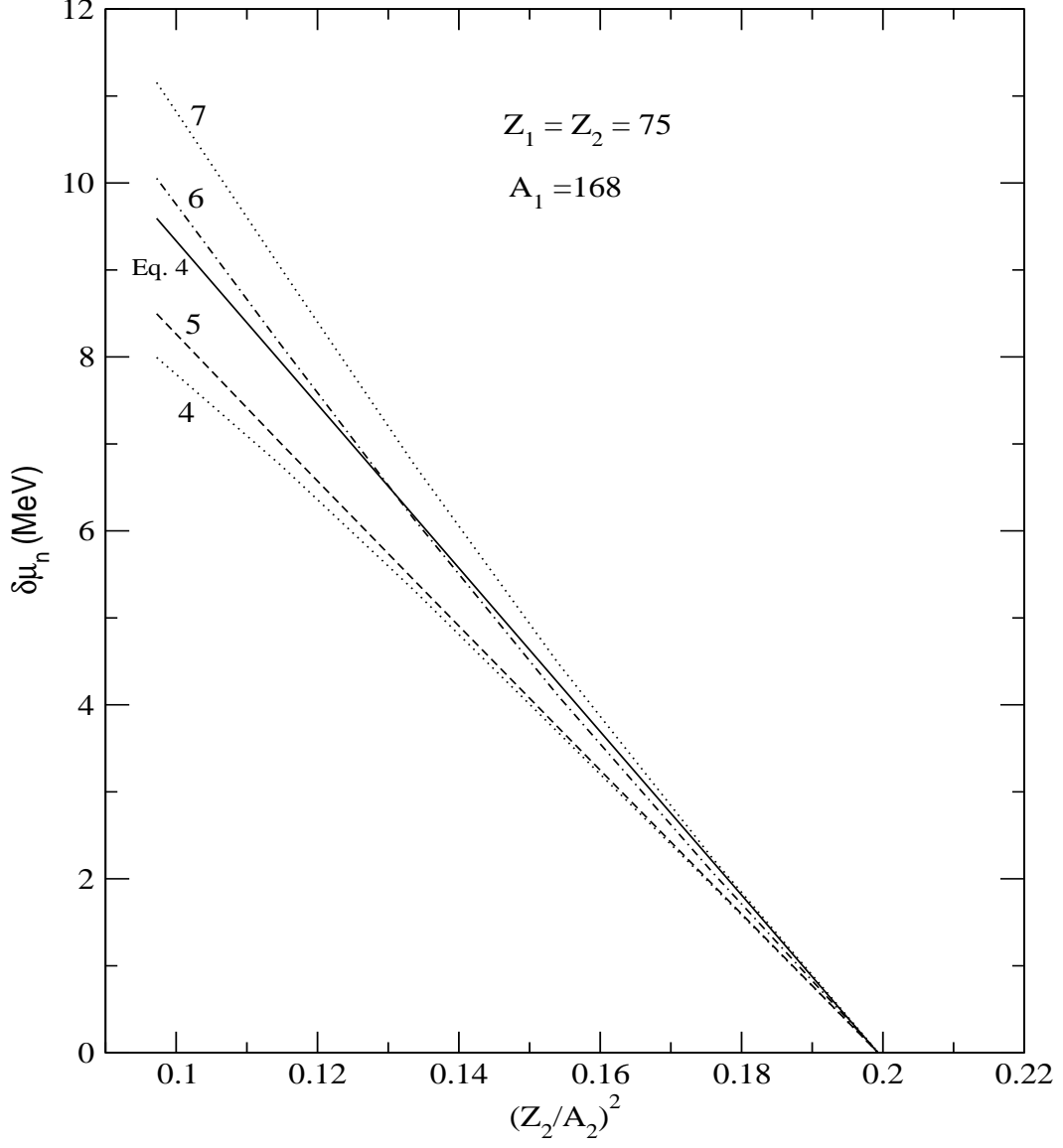


FIG. 4: This figure tests the linearity of $\delta\mu_n$ against $(Z_2/A_2)^2$ for fixed (Z_1/A_1) . Canonical model calculations are done for varying values of Z_2/A_2 . The calculations are done with the value of C_s at 23.5 MeV. The solid line is a plot of eq.(4) with $C_s=23.5$ MeV. Notice that at 4 or 5 MeV interpreting the canonical model result using eq.(4) will lead to an underestimation of the value of the underlying C_s and an overestimation at 7 MeV temperature. Linearity in thermodynamic calculation is not perfect but roughly correct in the temperature range displayed.

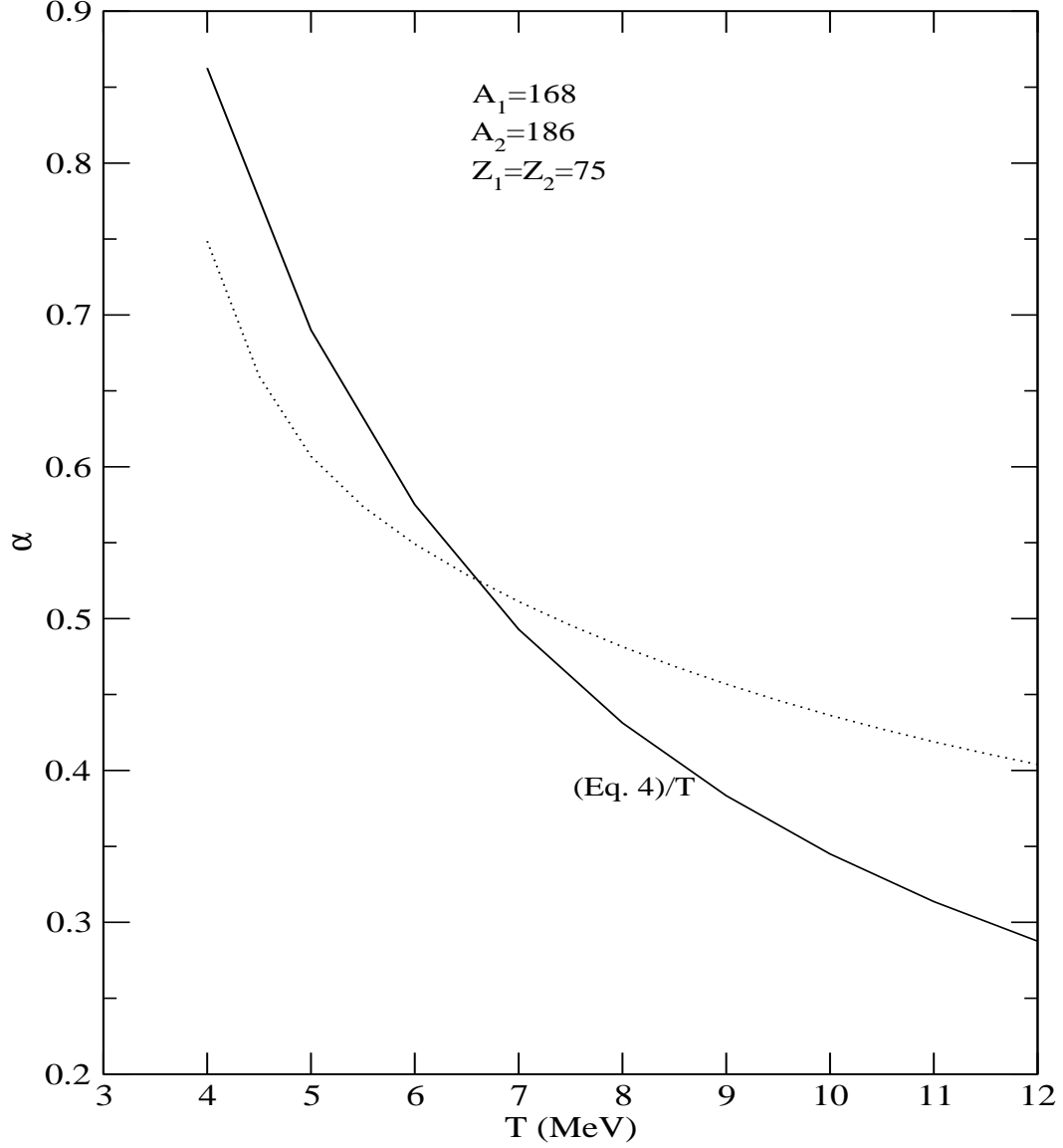


FIG. 5: The isoscaling parameter $\alpha = \delta\mu_n/T$ calculated in the canonical model (the dotted curve) is compared with the standard version $4(C_s/T)[(Z_1/A_1)^2 - (Z_2/A_2)^2]$ (solid curve). The thermodynamic model predicts that α becomes constant asymptotically whereas in standard parametrisation this would fall off like $1/T$.

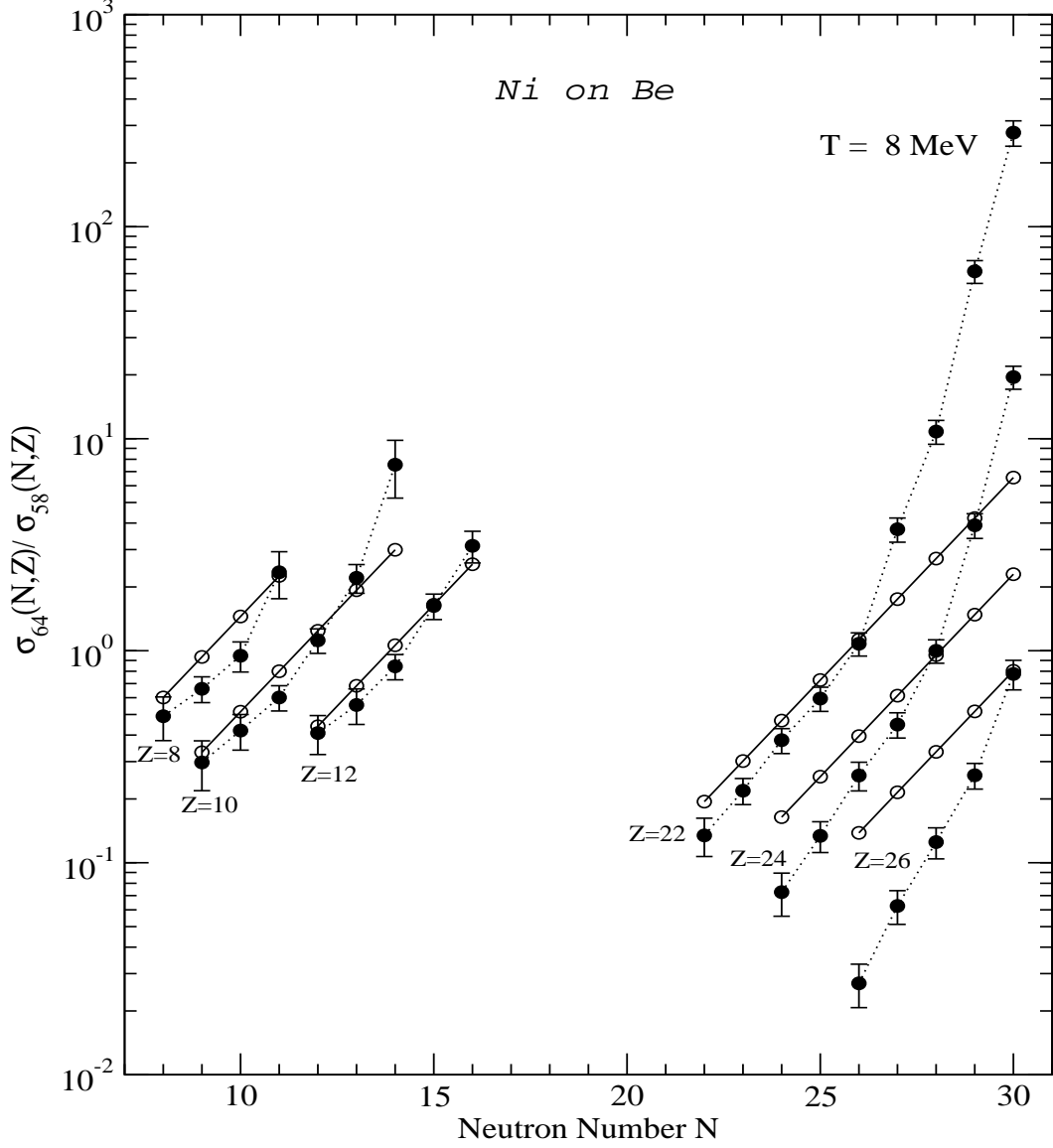


FIG. 6: Ratio of cross-sections of producing the nucleus (N,Z) where reaction 1 is ^{58}Ni on ^9Be and reaction 2 is ^{64}Ni on ^9Be , both at 140 MeV/n beam energy. Experimental data with error bars are compared with theoretical results from grand canonical ensemble (hollow points). Dotted lines are drawn through experimental points and solid lines through calculated points. For calculation the dissociating systems are taken to be Ni+Be. The constant C (eq.(42)) should be of the order 1 and in drawing the figure is taken to be 1. The value of the constant does not affect the slope of the log of the ratio. Notice that for large (N,Z) the slopes are no longer those of a straight line and that “average” slopes for small (N,Z) and large (N,Z) are very different in experiments but the same in grand canonical calculation.

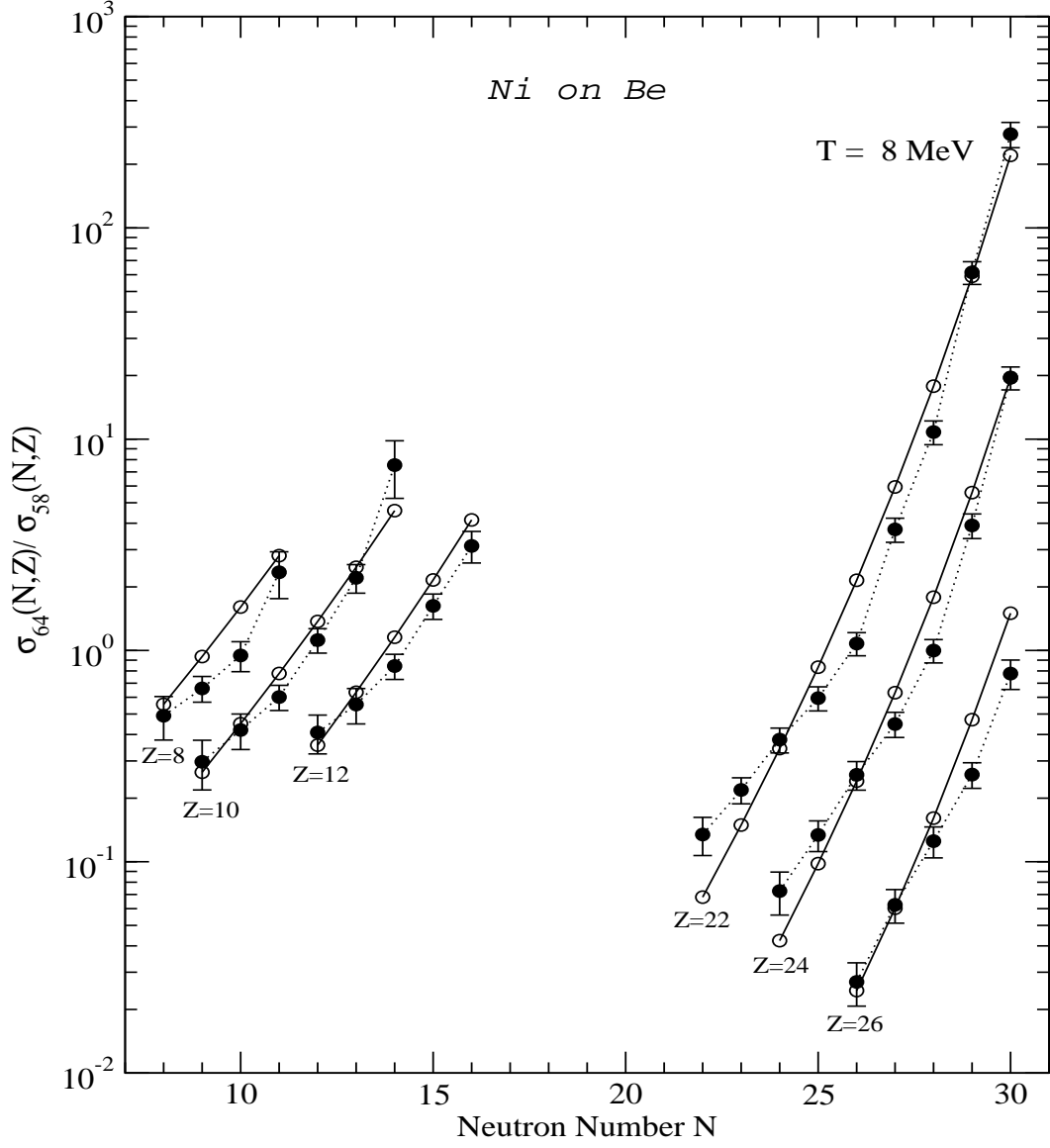


FIG. 7: The same as in Fig.6 except that the calculation is done in the canonical ensemble. Agreement with data is far superior compared to that in Fig.6.

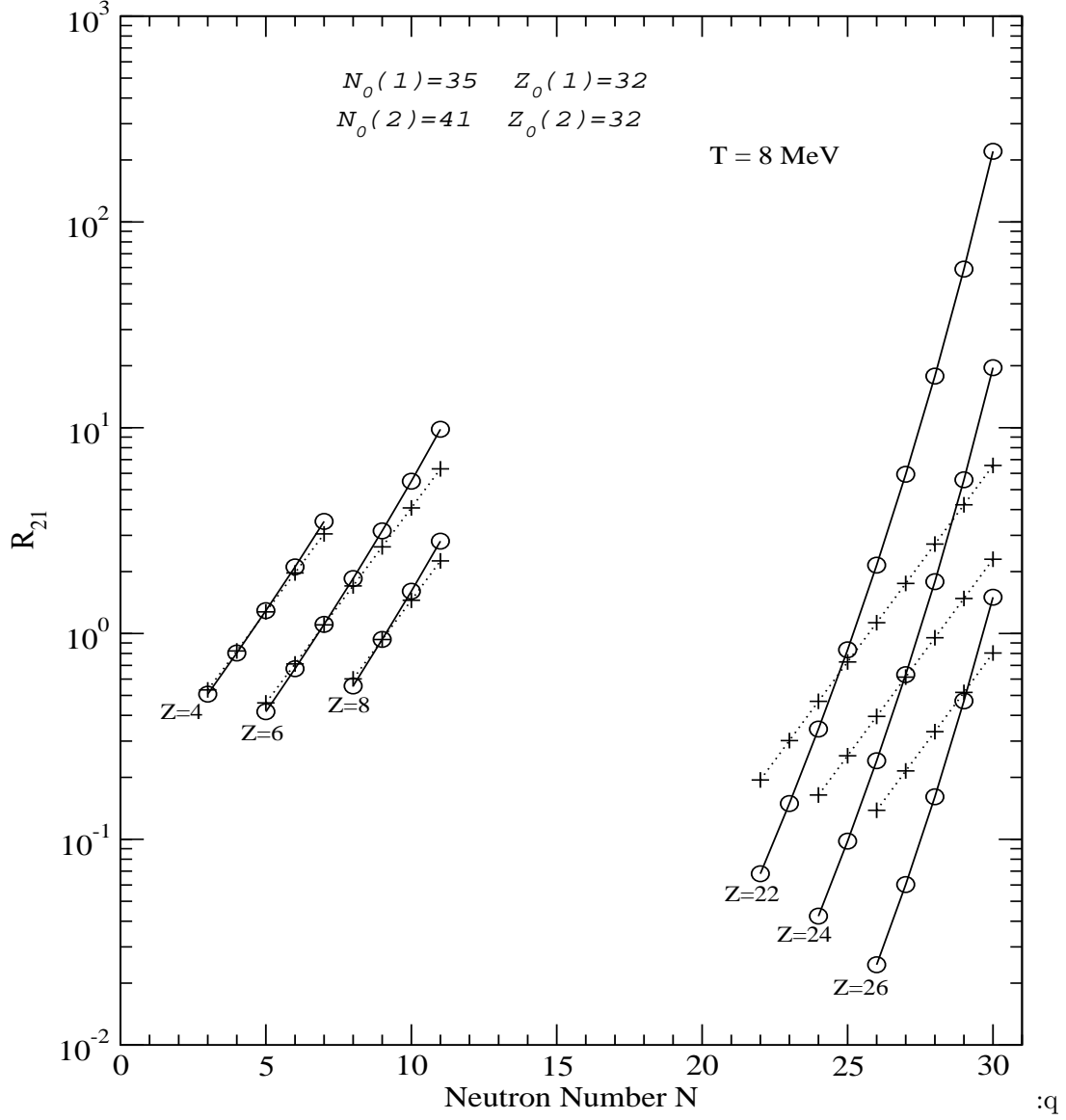


FIG. 8: Comparisons of R_{21} in canonical and grand canonical models. The solid lines are through points computed in the canonical model and the dotted lines are through points calculated in the grand canonical model. The dissociating systems are the same as in Figs. 6 and 7 and most of the points also appear in those figures. Here we show results for lower N, Z also to emphasize that for low N, Z agreement between canonical and grand canonical is very good (and for these isoscaling works) but that they differ widely for large N, Z . The grand canonical model should be discarded for large N, Z .

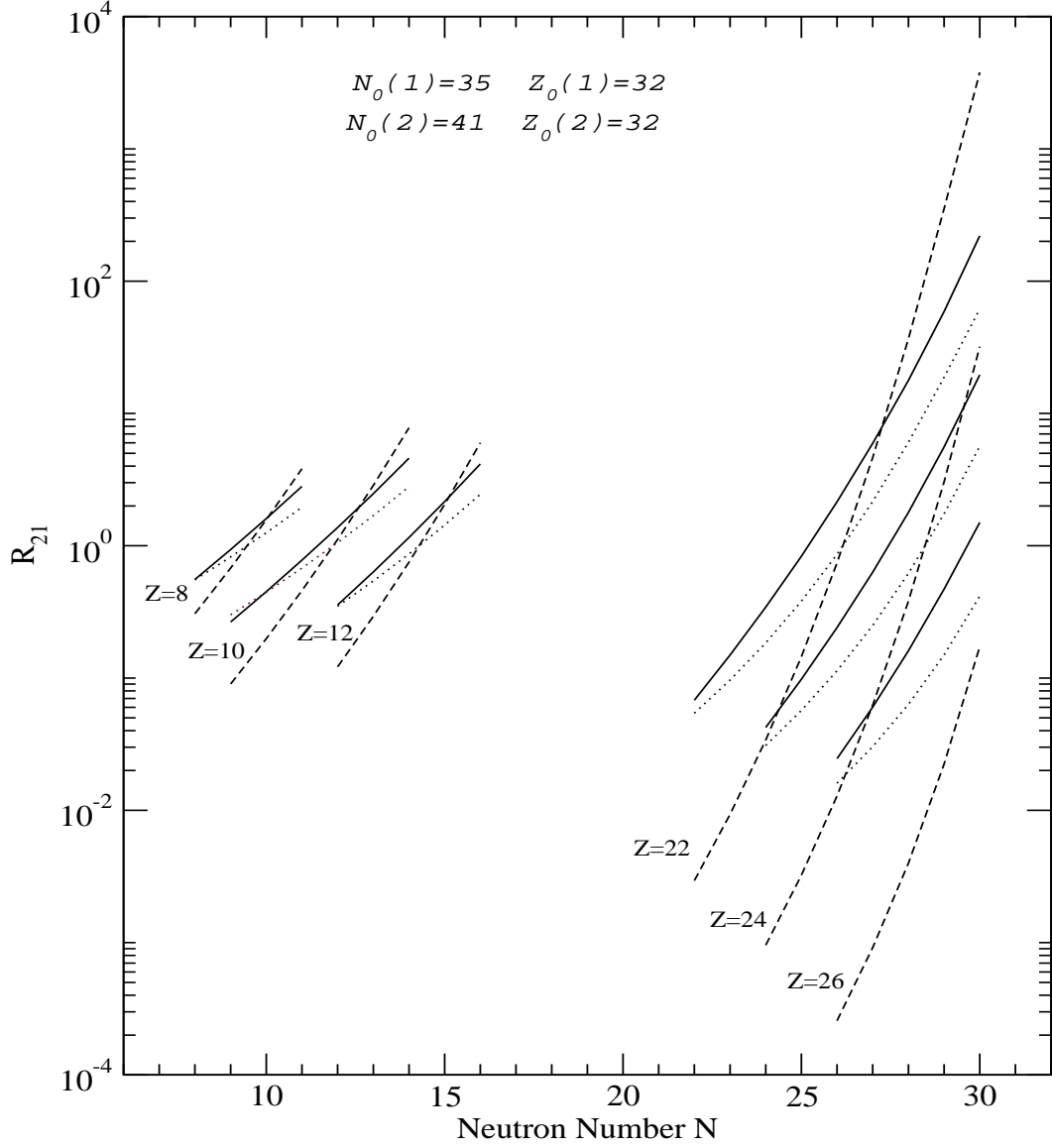


FIG. 9: The solid lines are canonical model results for R_{21} at temperature 8 MeV (no effects of secondary decay). This already fits the data quite well (Fig.7). For temperature 4.5 MeV we show two results. The dashed lines are the direct calculations (no corrections for decay). The slopes are much higher than the 8 MeV curves. The dotted curves include a phenomenological correction (see section IX) due to decay. It brings down the slope and mimics the raw calculation at 8 MeV (solid line here) and hence would fit the data reasonably well.